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## **Intrinsic and structural isotope effects in iron-based superconductors**

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**Abstract:** The currently available results of the isotope effect on the superconducting transition temperature  $T_c$  in Fe-based high-temperature superconductors (HTSs) are highly controversial. The values of the Fe isotope effect exponent  $\alpha_{Fe}$  for various families of Fe-based HTS were found to be as well positive, as negative, or even be exceedingly larger than the BCS value  $\alpha_{BCS} = 0.5$ . Here we emphasize that the Fe isotope substitution causes small structural modifications which, in turn, affect  $T_c$ . Upon correcting the isotope effect exponent for these structural effects, an almost unique value of  $\alpha_{Fe} = 0.35\text{--}0.4$  is observed for at least three different families of Fe-based HTS. © 2010 The American Physical Society

DOI: <https://doi.org/10.1103/PhysRevB.82.212505>

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ZORA URL: <https://doi.org/10.5167/uzh-45343>

Journal Article

Accepted Version

Originally published at:

Khasanov, R; Bendele, M; Bussmann-Holder, A; Keller, H (2010). Intrinsic and structural isotope effects in iron-based superconductors. *Physical Review. B, Condensed Matter and Materials Physics*, 82(21):212505.

DOI: <https://doi.org/10.1103/PhysRevB.82.212505>

# Intrinsic and structural isotope effects in Fe-based superconductors

R. Khasanov,<sup>1,\*</sup> M. Bendele,<sup>1,2</sup> A. Bussmann-Holder,<sup>3</sup> and H. Keller<sup>2</sup>

<sup>1</sup>Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland

<sup>2</sup>Physik-Institut der Universität Zürich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland

<sup>3</sup>Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany

The currently available results of the isotope effect on the superconducting transition temperature  $T_c$  in Fe-based high-temperature superconductors (HTS) are highly controversial. The values of the Fe isotope effect (Fe-IE) exponent  $\alpha_{\text{Fe}}$  for various families of Fe-based HTS were found to be as well positive, as negative, or even be exceedingly larger than the BCS value  $\alpha_{\text{BCS}} \equiv 0.5$ . Here we demonstrate that the Fe isotope substitution causes small structural modifications which, in turn, affect  $T_c$ . Upon correcting the isotope effect exponent for these structural effects, an almost unique value of  $\alpha \sim 0.35 - 0.4$  is observed for at least three different families of Fe-based HTS.

PACS numbers: 74.70.Xa, 74.62.Bf, 74.25.Kc

The isotope effect on the superconducting transition temperature  $T_c$  traditionally plays an important role in identifying the superconducting pairing mechanism. As a rule, an impact of the isotope substitution and, consequently, an involvement of the lattice degrees of freedom into the pairing mechanism are determined by comparing the isotope effect exponent  $\alpha = -(\Delta T_c / T_c) / (\Delta M / M)$  ( $M$  is the atomic mass) with the universal value  $\alpha_{\text{BCS}} \equiv 0.5$  as predicted within the framework of BCS theory of electron-phonon mediated superconductivity.

In conventional phonon mediated superconductors like simple metals, alloys, *etc.*  $\alpha$ , typically, ranges from 0.2 to 0.5, see, *e.g.*, Ref. 1 and references therein. The only exceptions are Ru and Zr exhibiting zero isotope effect and PdH(D) with  $\alpha_{\text{H(D)}} = -0.25$ .<sup>2</sup> The negative isotope effect of PdH(D) is explained, however, by the presence of strong lattice anharmonicity caused by the double-well potential in the proton (deuteron) bond distribution.<sup>3</sup> This was confirmed by neutron scattering data where the large zero point motion of H in comparison with that of Deuterium results in 20% change of the lattice force constants.<sup>4</sup> A similar finding exists in organic superconductors where the H(D) isotope effect changes sign as compared, *e.g.*, to <sup>34</sup>S, <sup>13</sup>C, and <sup>15</sup>N isotope replacements, see, *e.g.*, Ref. 5 and references therein. Again, an unusually strong anharmonic lattice dynamics are attributed to this observation.<sup>5,6</sup> The cuprate high-temperature superconductors (HTS) are characterized by a vanishingly small but positive isotope effect exponent in optimally doped compounds which increases in a monotonic way upon decreasing doping.<sup>7-14</sup> For the optimally doped cuprate HTS the smallest value of the oxygen-isotope exponent  $\alpha_{\text{O}} \simeq 0.02$  was obtained for YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7- $\delta$</sub>  and Bi<sub>2</sub>Sr<sub>2</sub>Ca<sub>2</sub>Cu<sub>3</sub>O<sub>10+ $\delta$</sub> , while it reaches  $\alpha_{\text{O}} \simeq 0.25$  for Bi<sub>2</sub>Sr<sub>1.6</sub>La<sub>0.4</sub>CuO<sub>6+ $\delta$</sub> .<sup>7-9,13,14</sup> In addition, it was demonstrated that in underdoped materials  $\alpha_{\text{O}}$  exceeds substantially the BCS limit  $\alpha_{\text{BCS}} \equiv 0.5$ .<sup>8,10,14</sup> It is important to note here that the values of both, the oxygen and the copper isotope exponents in cuprate HTS are *always* positive. Similar tendencies, with the only few above mentioned exceptions, are realized in a case of conventional phonon mediated superconductors.

Since the discovery of superconductivity in Fe-based compounds few attempts to measure the isotope effect on

$T_c$  in these materials were made. Currently we are aware of four papers reporting, however, rather contradictory results.<sup>15-18</sup> Liu *et al.*<sup>15</sup> and Khasanov *et al.*<sup>18</sup> have found a *positive* Fe isotope effect (Fe-IE) exponent  $\alpha_{\text{Fe}}$  for Ba<sub>0.6</sub>K<sub>0.4</sub>Fe<sub>2</sub>As<sub>2</sub>, SmFeAsO<sub>0.85</sub>F<sub>0.15</sub>, and FeSe<sub>1- $x$</sub>  with the corresponding values  $\alpha_{\text{Fe}} = 0.34(3)$ ,  $0.37(3)$ , and  $0.81(15)$ , respectively. Note that  $\alpha_{\text{Fe}} = 0.81(15)$  for FeSe<sub>1- $x$</sub>  exceeds grossly the BCS value. In the other two studies Shirage *et al.* have reported a *negative*  $\alpha_{\text{Fe}} = -0.18(3)$  and  $-0.024(15)$  for Ba<sub>0.6</sub>K<sub>0.4</sub>Fe<sub>2</sub>As<sub>2</sub><sup>16</sup> and SmFeAsO<sub>1- $y$</sub> ,<sup>17</sup> respectively. These controversial results are unlikely to stem from different pairing mechanisms to be realized in different Fe-based superconductors. Especially, in the case of Ba<sub>0.6</sub>K<sub>0.4</sub>Fe<sub>2</sub>As<sub>2</sub>, nominally identical samples were isotope replaced with one exhibiting a positive<sup>15</sup> and the other a negative isotope exponent.<sup>16</sup> Note, that the sign reversed isotope exponent seen by Shirage *et al.*<sup>16,17</sup> was attributed to multi-band superconductivity with different pairing channels, namely a phononic one and an antiferromagnetic (AF) fluctuation dominated one.<sup>19</sup> On the other hand a multi-band model cannot exhibit *any* sign reversed isotope exponent even if solely AF fluctuations were the pairing glue.<sup>20</sup>

In the present study we demonstrate that the very controversial results for  $\alpha_{\text{Fe}}$  are caused by small structural changes occurring simultaneously with the Fe isotope exchange. As such, we decompose the Fe-IE exponent into one related to the structural changes  $\alpha_{\text{Fe}}^{\text{str}}$  and the genuine (intrinsic) one  $\alpha_{\text{Fe}}^{\text{int}}$  to arrive at:

$$\alpha_{\text{Fe}} = \alpha_{\text{Fe}}^{\text{int}} + \alpha_{\text{Fe}}^{\text{str}}. \quad (1)$$

By comparing the c-axis lattice constants for the pairs of isotopically substituted samples we observe that  $\alpha_{\text{Fe}}^{\text{str}}$  is negative for Ba<sub>0.6</sub>K<sub>0.4</sub>Fe<sub>2</sub>As<sub>2</sub> and SmFeAsO<sub>1- $y$</sub>  studied by Shirage *et al.* in Refs. 16 and 17, positive for FeSe<sub>1- $x$</sub>  from Ref. 18 and close to 0 for Ba<sub>0.6</sub>K<sub>0.4</sub>Fe<sub>2</sub>As<sub>2</sub> and SmFeAsO<sub>0.85</sub>F<sub>0.15</sub> measured in Ref. 15. By taking into account the sign of  $\alpha_{\text{Fe}}^{\text{str}}$  we arrive at the conclusion that  $\alpha_{\text{Fe}}^{\text{int}}$  is positive for all so far studied Fe-based HTS.

Our motivation to separate the isotope coefficient into the above mentioned two components, see Eq. (1), stems from the fact that superconductivity in these compounds is intimately related to small structural changes as re-

TABLE I: Summary of Fe isotope effect studies for  $\text{FeSe}_{1-x}$  Ref. 18,  $\text{SmFeAsO}_{0.85}\text{F}_{0.15}$  and  $\text{Ba}_{0.6}\text{K}_{0.4}\text{Fe}_2\text{As}_2$  Ref. 15,  $\text{Ba}_{0.6}\text{K}_{0.4}\text{Fe}_2\text{As}_2$  Ref. 16 and  $\text{SmFeAsO}_{1-x}$  Ref. 17. The parameters are:  $T_c$  – superconducting transition temperature for the sample with the natural Fe isotope ( $^{\text{nat}}\text{Fe}$ );  $\alpha_{\text{Fe}}$  – Fe isotope effect exponent;  $c$  – the c-axis lattice constant for the sample with the lighter ( $^{\text{light}}\text{Fe}$ ) and the heavier ( $^{\text{heavy}}\text{Fe}$ ) Fe isotope;  $\Delta c/c$  – the relative shift of the c-axis constant caused by the Fe isotope substitution;  $\alpha_{\text{Fe}}^{\text{str}}$  and  $\alpha_{\text{Fe}}^{\text{int}}$  – the structural and the intrinsic contributions to  $\alpha_{\text{Fe}}$ . See text for details.

Sample	Reference	$T_c(^{\text{nat}}\text{Fe})$ (K)	$\alpha_{\text{Fe}}$	c-axis( $^{\text{light}}\text{Fe}$ ) (Å)	c-axis( $^{\text{heavy}}\text{Fe}$ ) (Å)	$\Delta c/c$	$\alpha_{\text{Fe}}^{\text{str}}$	$\alpha_{\text{Fe}}^{\text{int}}$
$\text{FeSe}_{1-x}$	Ref. 18	8.21(4)	0.81(15)	5.48683(9)	5.48787(9)	$> 0$	$\simeq 0.4$	$\simeq 0.4$
$\text{Ba}_{0.6}\text{K}_{0.4}\text{Fe}_2\text{As}_2$	Ref. 15	37.30(2)	0.37(3)	13.289(7)	13.288(7)	$\sim 0$	$\sim 0$	$\sim 0.35$
$\text{Ba}_{0.6}\text{K}_{0.4}\text{Fe}_2\text{As}_2$	Ref. 16	37.78(2)	-0.18(3)	13.313(1)	13.310(1)	$< 0$	$\sim -0.5$	–
$\text{SmFeAsO}_{0.85}\text{F}_{0.15}$	Ref. 15	41.40(2)	0.34(3)	8.490(2)	8.491(2)	$\sim 0$	$\sim 0$	$\sim 0.35$
$\text{SmFeAsO}_{1-y}$	Ref. 17	54.02(13)	-0.024(15)	8.4428(8)	8.4440(8)	$\gtrsim 0$	$< 0$	–

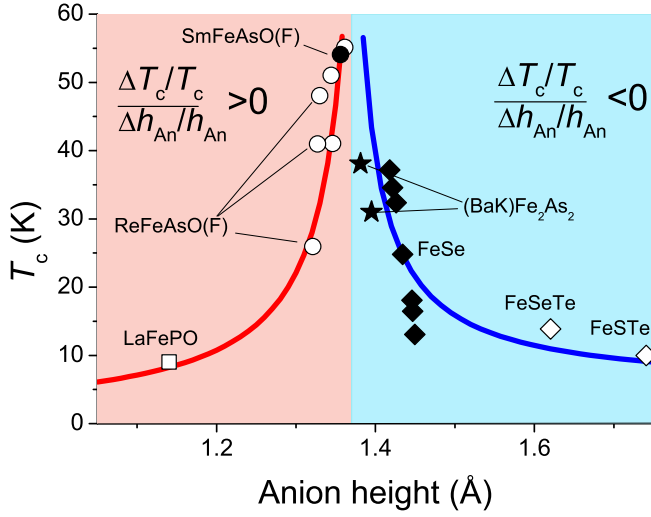


FIG. 1: (color online) Dependence of the superconducting transition temperature  $T_c$  on the height of the anion atom ( $h_{\text{An}}$ ,  $\text{An}=\text{As}, \text{Se}, \text{P}$ ) for various families of Fe-based HTS, after Mizuguchi *et al.*<sup>21</sup>). The closed symbols represent the samples which are relevant for the present study. The lines are guided for the eye. The red(blue) area represents part of  $T_c$  vs.  $h_{\text{An}}$  diagram where  $T_c$  increases(decreases) with increasing  $h_{\text{An}}$ .

ported in various works. As an example, we mention the strong nonlinear dependence of the superconducting transition temperature on the anion atom height ( $h_{\text{An}}$ ,  $\text{An}=\text{As}, \text{P}, \text{or Se}$ ) with a sharp maximum of  $T_c$  at  $h_{\text{An}} \simeq 1.38$  Å, see Mizuguchi *et al.*<sup>21</sup> and Fig. 1. The influence of the Fe isotope substitution on the crystal structure, on the other hand, was first considered by Granath *et al.*<sup>22</sup> based on the results of Raman studies of  $\text{CaFeAsO}_{1-x}$  and  $\text{NdFeAsO}_{1-x}$  and further confirmed by Khasanov *et al.*<sup>18</sup> in neutron powder diffraction experiments on  $^{54}\text{Fe}$  to  $^{56}\text{Fe}$  substituted  $\text{FeSe}_{1-x}$ .

The c-axis lattice constants for the pairs of Fe isotope substituted samples  $\text{Ba}_{0.6}\text{K}_{0.4}\text{Fe}_2\text{As}_2$ ,  $\text{SmFeAsO}_{0.85}\text{F}_{0.15}$ ,  $\text{SmFeAsO}_{1-y}$ , and  $\text{FeSe}_{1-x}$  studied in Refs. 15–18 are summarized in Table I. The choice

of the c-axis lattice constant as the relevant quantity in deriving the structural isotope effect might appear to be rather arbitrary since  $T_c$  is influenced by all structural details, namely tetrahedral angle, a-axis lattice constant, internal bond lengths, *etc.* However, the c-axis lattice constant provides a very sensitive probe since its compression(expansion) is directly accompanied by the corresponding variation of the distance from the Fe-planes to the above(below) lying anions<sup>23–25</sup> which, in turn, is a well characterized property for many Fe-based compounds.<sup>21</sup> From Table I it is obvious that in  $\text{Ba}_{0.6}\text{K}_{0.4}\text{Fe}_2\text{As}_2$  and  $\text{SmFeAsO}_{0.85}\text{F}_{0.15}$ <sup>15</sup> the c-axis constants are the same within the experimental error for both isotopically substituted sets of the samples.<sup>26</sup> In  $\text{FeSe}_{1-x}$ <sup>18</sup> the c-axis constant is larger, while in  $\text{Ba}_{0.6}\text{K}_{0.4}\text{Fe}_2\text{As}_2$ <sup>16</sup> it is smaller for the sample with the heavier Fe isotope. In  $\text{SmFeAsO}_{1-y}$ , studied by Shirage *et al.*,<sup>17</sup> both c-axis lattice constants seem to coincide within the experimental resolution. However, since the difference between them is 1.5 times larger than one standard deviation, it is conceivable to attribute an increase in the c-axis lattice constant in  $\text{SmFeAsO}_{1-y}$  with the heavier Fe isotope.

The use of the empirical  $T_c$  vs.  $h_{\text{An}}$  relation from Ref. 21 combined with the intrinsic relation of the proportionality between the c-axis constant and the anion atom height ( $\Delta c \propto \Delta h_{\text{An}}$ , see Refs. 23–25) enables us to determine the sign of the structurally related shift of  $T_c$  induced by isotopic exchange. By defining the shift of a given quantity  $X$  as  $\Delta X/X = ({}^{\text{light}}\text{Fe} X - {}^{\text{heavy}}\text{Fe} X)/{}^{\text{heavy}}\text{Fe} X$  and following Mizuguchi *et al.*<sup>21</sup>, see also Fig. 1, the sign of  $(\Delta T_c/T_c)/(\Delta h_{\text{An}}/h_{\text{An}})$  is positive for  $\text{SmFeAsO}(\text{F})$  as well as for various Fe-based HTS belonging to  $\text{ReFeAsO}(\text{F})$  family ( $\text{Re}=\text{Nd}, \text{Ce}, \text{La}$ ) and negative for  $(\text{BaK})\text{Fe}_2\text{As}_2$  and  $\text{FeSe}_{1-x}$ . Consequently the change of the c-axis constant caused by Fe isotope substitution as presented in Table I results in an additional structurally related shift of  $T_c$  being positive for  $\text{FeSe}_{1-x}$ ,<sup>18</sup> negative for  $\text{Ba}_{0.6}\text{K}_{0.4}\text{Fe}_2\text{As}_2$  and  $\text{SmFeAsO}_{1-y}$ ,<sup>16,17</sup> and close to 0 for  $\text{Ba}_{0.6}\text{K}_{0.4}\text{Fe}_2\text{As}_2$  and  $\text{SmFeAsO}_{0.85}\text{F}_{0.15}$ .<sup>15</sup> It is rather remarkable that the corresponding “structural” Fe-IE exponents  $\alpha_{\text{Fe}}^{\text{str}}$  would

lead to the shift of genuine (intrinsic)  $\alpha_{\text{Fe}}^{\text{int}}$  in the direction of 0.35–0.4, see Fig. 2.

Note that the above mentioned discussion allows only to determine the sign of the structurally related isotope effect but not the absolute value. The reasons are the following. First, the relative change of the c-axis constant is proportional, but not identical to the one of  $h_{\text{An}}$ . As an example,  $^{56}\text{Fe}$  to  $^{54}\text{Fe}$  isotope substitution in  $\text{FeSe}_{1-x}$  leads to an increase of the c-axis constant by approximately 0.02%, while the change of the Se height amounts to  $\simeq 0.22\%$ , see Ref. 18. Second, the height of the anion atom is clearly not the only parameter which is crucial for  $T_c$  of Fe-based HTS as already mentioned above. However, the lack of a consistent structural characterization limits this study to a single parameter which was emphasized to be of uppermost relevance to  $T_c$ .

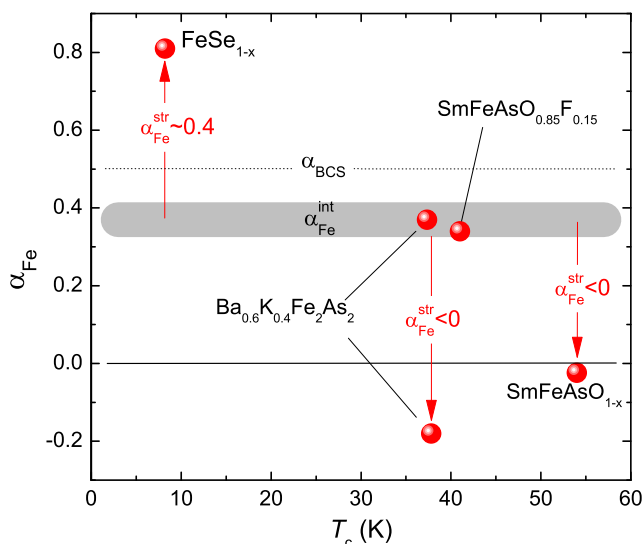


FIG. 2: (color online) Fe isotope effect exponent  $\alpha_{\text{Fe}}$  as a function of the superconducting transition temperature  $T_c$  for the samples considered in the present study:  $\text{FeSe}_{1-x}$  Ref. 18,  $\text{Ba}_{0.6}\text{K}_{0.4}\text{Fe}_2\text{As}_2$  and  $\text{SmFeAsO}_{0.85}\text{F}_{0.15}$  Ref. 15,  $\text{Ba}_{0.6}\text{K}_{0.4}\text{Fe}_2\text{As}_2$  Ref. 16, and  $\text{SmFeAsO}_{1-x}$  Ref. 17. Arrows indicate the direction of the shift from the “intrinsic” Fe-isotope effect exponent  $\alpha_{\text{Fe}}^{\text{int}} \sim 0.35 - 0.4$  caused by the structural effects.  $\alpha_{\text{BCS}} \equiv 0.5$  is the BCS value for electron-phonon mediated superconductivity. See text for details

The analysis of the structural data together with the dependence of  $T_c$  on Se height in  $\text{FeSe}_{1-x}$ , as well as on Se(Te)–Fe–Se(Te) angle and the a-axis constant in  $\text{FeSe}_{1-y}\text{Te}_y$  for  $y \leq 0.5$  admits to extract the “structural” Fe isotope effect exponent  $\alpha_{\text{Fe}}^{\text{str}} \simeq 0.4$  for  $^{56}\text{Fe}$  to  $^{54}\text{Fe}$  substituted  $\text{FeSe}_{1-x}$  samples.<sup>18</sup> The absence of precise structural data complicates the precise analysis as

outlined in Refs. 15–17. However, a zero, within the experimental accuracy, Fe isotope shift of the c-axis lattice constant for  $\text{Ba}_{0.6}\text{K}_{0.4}\text{Fe}_2\text{As}_2$  as reported by Liu *et al.*<sup>15</sup> is a clear indication that no structural effect is present for this particular set of the samples. Consequently, the negative isotope effect exponent  $\alpha_{\text{Fe}} \simeq -0.18$  obtained for nominally identically doped  $\text{Ba}_{0.6}\text{K}_{0.4}\text{Fe}_2\text{As}_2$  by Shirage *et al.*<sup>16</sup> stems from summing both effects, *i.e.*,  $-0.18(\alpha_{\text{Fe}}) = 0.35(\alpha_{\text{Fe}}^{\text{int}}) - 0.52(\alpha_{\text{Fe}}^{\text{str}})$ , see Eq. (1). It is important to recognize that for  $\text{SmFeAsO}(\text{F})$  a similar analysis is impossible since samples with different doping levels (different  $T_c$ ’s, see Table I and Fig. 2) were studied in Refs. 15 and 17.

Recently Bussmann-Holder *et al.*<sup>27</sup> investigated a multiple gap scenario of superconductivity in Fe-based HTS with the aim to search for possible sources of the isotope effect on  $T_c$ . Typical phonon mediated scenarios were contrasted to polaronic effects and found to have very different impacts on the isotope effect. While phonon mediated superconductivity slightly suppresses the isotope effect as compared to the BCS value  $\alpha_{\text{BCS}} \equiv 0.5$ , polaronic effects can largely enhance it. The scenario of electron-phonon mediated superconductivity within the dominant gap channel predicts a  $T_c$  independent isotope effect with the  $\alpha$  value being slightly smaller than 0.5 thus agreeing rather well with that observed for  $\text{FeSe}_{1-x}$ ,<sup>18</sup>  $\text{Ba}_{0.6}\text{K}_{0.4}\text{Fe}_2\text{As}_2$ ,<sup>15,16</sup> and  $\text{SmFeAsO}_{0.85}\text{F}_{0.15}$ .<sup>15</sup> Indeed, for these particular samples, which belong to 3 different families of Fe-based HTS and have  $T_c$ ’s between 8 and 44 K, the “intrinsic” Fe isotope exponent is almost constant with  $\alpha_{\text{Fe}}^{\text{int}} \sim 0.35 - 0.4$ , see Table I and Fig. 2. As such, the independent on  $T_c$  value of  $\alpha_{\text{Fe}}^{\text{int}}$  would suggest  $\alpha_{\text{Fe}}^{\text{str}} \sim -0.4$  for  $\text{SmFeAsO}_{1-x}$  studied by Shirage *et al.*<sup>17</sup>

To conclude, the currently available Fe isotope effect data on the superconducting transition temperature  $T_c$  for various Fe-based HTS were reanalyzed by separating the measured Fe-IE exponent  $\alpha_{\text{Fe}}$  into a structural and an intrinsic (unrelated to the structural changes) component. Accounting for the empirical relation between  $T_c$  and the anion atom height  $h_{\text{An}}$ <sup>21</sup> we have demonstrated that the structural contribution to the Fe-IE exponent is negative for  $\text{Ba}_{0.6}\text{K}_{0.4}\text{Fe}_2\text{As}_2$  and  $\text{SmFeAsO}_{1-x}$  studied by Shirage *et al.*,<sup>16,17</sup> positive for  $\text{FeSe}_{1-x}$ ,<sup>18</sup> and close to 0 for  $\text{SmFeAsO}_{0.85}\text{F}_{0.15}$  and  $\text{Ba}_{0.6}\text{K}_{0.4}\text{Fe}_2\text{As}_2$  measured by Liu *et al.*<sup>15</sup> By taking such corrections into account we infer that the value of the genuine Fe-IE exponent is close to  $\alpha_{\text{Fe}}^{\text{int}} \sim 0.35 - 0.4$  for compounds belonging to at least three different families of Fe-based HTS. We are convinced that the analysis presented in our paper helps in clarifying the existing controversy on the isotope effect in Fe-based superconductors.

\* Corresponding author: rustem.khasanov@psi.ch

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